Mens Agitat, vol. 15 (2020)43-45 . ISSN 1809-4791

Superheavy elements (Z = 100 to 109) treated as calcium clusters: ionization energies

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Abstract In the present work, it is shown that the first ionization energies for super-heavy elements (Z= 100-109) can be calculated by a semi-empirical method, if the super-heavy elements are treated (modelled) as calcium clusters. The values calculated in the present work are in good agreement compared with those from literature (modelling the super-heavy elements themselves, based on relativistic quantum mechanics).

Keywords: Super-heavy elements, calcium clusters, ionization energy, semi-empirical

INTRODUCTION

The search for new chemical elements have resulted in the discovery of the elements 111-118. Since their chemical and physical properties are difficult of even impossible to be accessed/measured directly, the so-called super-heavy elements have been the subject of a lot of theoretical investigations and some works have been dedicated to estimate/predict the properties of such elements [1-6].

Taking into account their higher Z values, trustable calculations involving the properties of super-heavy elements must, necessarily, include the relativistic contributions [7]. However, even today, with the development of faster computers, such calculations are not so easy from an exclusively computational point of view, and only a relatively few researchers/groups are really able/dedicated to them.

In the present work, is shown that the first ionization energies for super-heavy elements (Z= 100-109) can be calculated by a semi-empirical method, if the super-heavy elements are treated as calcium clusters. The values calculated in the present work are compared with those from literature (mainly based on relativistic quantum mechanics calculations) as well experimental values, when available.

METHODOLOGY

All calculations were performed by using Spartan [8]. The calcium clusters were modelled as six membered rings. Since calcium has Z= 20, five calcium atoms were taken, and another element was "summed up" in order to provide a total of protons equals to the desired element. Hence, for element 103, for example, five calcium (Z= 20) atoms and one lithium (Z= 3) atom were employed, and the cluster Ca_5Li has a total of 103 protons, as the element 103. The total number of neutrons is not the same, of course, but is considered here that only the elements charged particles affect the cluster energy levels.

The choice of calcium as the main clusters "building block" was not aleatory: calcium was chose taking into account that ^{40}Ca has a closed nuclear shell with protons and neutrons with the so called "magic configuration", been close to the line of stability [9]. Furthermore, calcium has been employed as "building block" for experimental super-

heavy elements synthesis since calcium is element 20, and calcium plus americium (element 95) yielded element 115, calcium plus curium (element 96) yielded element 116, and so on [10].

All clusters were modelled as neutrals or +1 cations, with the corresponding number of unpaired electrons.

All calculations were performed by semi-empirical (PM6) method. The SE-PM6 approach was chose taking into account its minor computation time consuming and its reliability for calculations involving inorganic systems, as verified for PtF_6 [11] and tin borates [12]. The only exception was the cluster Ca_5He^+, since PM6 method do not support He. For such cluster, Hartree-Fock (G-3111 + G**) method was employed.

RESULTS AND DISCUSSION

The obtained results are summarized in Table 1 and compared with calculated values from literature (mainly based on relativistic quantum chemical calculations) and experimental values [13], when available. The obtained equilibrium (minimum energy) structure to Ca_5 ("emulating" element 100) cluster is shown in Figure 1.

Table 1. First ionization energies (eV) for super-heavy elements modelled as calcium clusters.

Element	Z	Modelled cluster	IE/eV (cluster)	IE/eV (ref. values)
Fm	100	Ca_5 Ca_5^+	4.30 8.70 6.50*	6.50[d]
Md	101	Ca_5H Ca_5H^+	5.78 7.40 6.59*	6.58[d]
No	102	Ca_5He^+	6.70	6.65[d]
Lr	103	Ca_5Li Ca_5Li^+	5.76 7.65 6.71*	4.96[e] 4.96[c]
Rf	104	Ca_5Be Ca_5Be^+	4.52 9.04 6.78*	6.01[a] 6.50[b]
Db	105	Ca_5B^+	7.12	6.9[a]
Sg	106	Ca_5C^+	8.44	7.8[a]
Bh	107	Ca_5N^+	7.12	7.7[a]
Hs	108	Ca_5O^+	7.85	7.6[a]
Mt	109	Ca_5F^+	7.33	8.7[a]

*Mean value of the IE calculated to the neutral and cationic (+) cluster; [a]Ref. 9; [b]Based on estimated Clementi effective nuclear charges (Ref. 5); [c](Ref. 13); [d]CRC Handbook (Ref. 14); [e]Experimental value (Ref. 13);

As can be verified, the SE results are (with exception of element 103) in good (sometimes very good) agreement with the relativistic quantum chemical ones, showing that the employed approach is suitable/reliable. Of course, from times to times, some calculations are improved and a specific value for a given element can change a little form one work to another, but the main result, ie., the agreement between the SE (for calcium clusters) and relativistic (for the elements themselves) values remains.

From elements 100-104 (with exception of No) the "correct" (taking into account a reference value form literature) ionization energy value is the mean of the value calculated ones to the respective uncharged and cationic (+1) clusters.

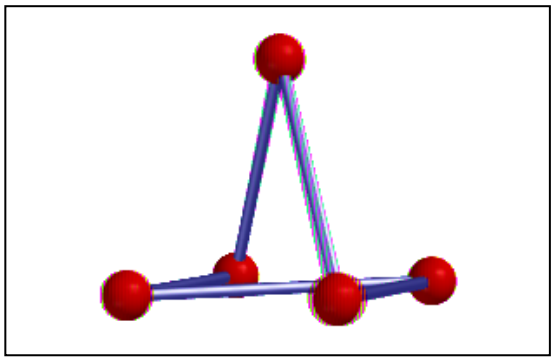

Fig. 1. Ca_5 cluster structure

This fact suggests that for such elements the "correct" energy level of the valence electron is a mean value of the uncharged and +1 cluster energy levels. In other words, the energy for the valence electron of the super-heavy element is a mean of the HOMO energies for the respective uncharged and cationic (+1) calcium cluster.

Curiously, this happens to the "lighter" (100, 101, 103 and 104 elements) but not the "heavier" 105-109 elements, suggesting that SE methods (calcium clusters) can provide trustable results (that is, comparable to those provided by the relativistic methods -the super-heavy elements themselves) as better as heavier is the considered element.

Of course, only the a profound and detailed analysis of the physical/mathematical "idiosyncrasies" of both theoretical approach can really provide a good explanation for such phenomena.

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